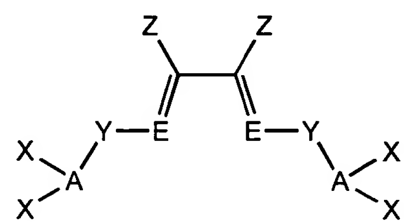
WHAT IS CLAIMED IS:

1. A catalyst composition for use in an olefin polymerization process, the catalyst composition comprising:

a late transition metal selected from the group consisting of IUPAC convention Group 7 (Mn column), Group 8 (Fe column), Group 9 (Co column), Group 10 (Ni column) and Group 11 (Cu column) transition metals; and

a ligand complexed with the late transition metal, the ligand being characterized by the general formula:



wherein each E is an electronegative atom capable of donating electrons to the late transition metal;

each Y is a linking group independently selected from the group consisting of -O-, -NR-, -CR_2-, -S-, -PR-, -SiR_2-, and -G$(CR_2)_m$-, where each R is a substituent independently selected from the group consisting of H, halide, alkyl, substituted alkyl, heteroalkyl, aryl, substituted aryl, and heteroaryl, and where one or more R substituents can be incorporated in a ring structure, G is selected from the group consisting of O, N, and CR_2, and m is an integer greater than or equal to 1;

each A is a Lewis acid;

each X is an electron-withdrawing group independently selected from the group consisting of

Cl, F, Br, I, CF_3, C_6F_5, H, alkyl, C_6H_5, C_6R_5, and CR_3, where each R is a substituent independently selected from the group consisting of H, halide, alkyl, substituted alkyl, heteroalkyl, aryl, substituted aryl, and heteroaryl, and where one or more R substituents can be incorporated in a ring structure;

each Z is a substituent independently selected from the group consisting of H, halide, alkyl, substituted alkyl, heteroalkyl, aryl, substituted aryl, and heteroaryl, where one or more of X, Y and/or Z can be incorporated in a ring structure;

wherein the late transition metal is also complexed with one or more additional ligands selected from the group consisting of ligands that are capable of adding to an olefin in a polymerization process and ligands that are capable of being displaced by the olefin.

2. The composition of claim 1, wherein:

each E is independently selected from the group consisting of N and P;

3. The composition of claim 1, wherein:

each A is independently independently selected from the group consisting of Al, B, Ga, In, Tl, Sc, Y, La and Lu.

4. The composition of claim 1, wherein:

the late transition metal is nickel, palladium or platinum.

5. The composition of claim 1, wherein:

the late transition metal is nickel, palladium or platinum;

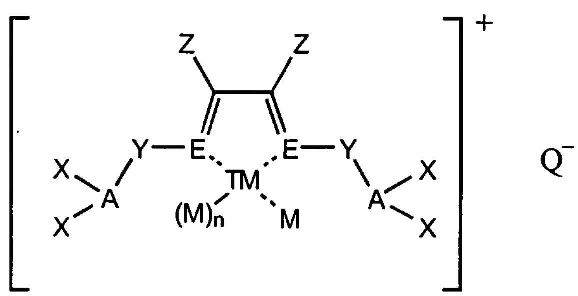
A is aluminum or scandium;

Y is -O-, -S-, or $-CH_2-$;

X is Cl, F, CF_3 or H; and

Z is H.

6. A compound characterized by the general formula:



wherein TM is a late transition metal selected from the group consisting of Groups 7-11 transition metals;

each E is an electronegative atom capable of donating electrons to the late transition metal;

each Y is a linking group independently selected from the group consisting of -O-, -NR-, $-CR_2-$, -S-, -PR-, $-SiR_2-$, and $-G(CR_2)_m-$, where each R is a substituent independently selected from the group consisting of H, halide, alkyl, substituted alkyl, heteroalkyl, aryl, substituted aryl, and heteroaryl, and where one or more R substituents can be incorporated in a ring structure, G is selected from the group consisting of O, N, and CR_2, and m is an integer greater than or equal to 1;

each A is a Lewis acid;

each X is an electron-withdrawing group independently selected from the group consisting of Cl, F, Br, I, CF_3, C_6F_5, H, alkyl, C_6H_5, C_6R_5, and CR_3, where each R is a substituent independently selected from the group consisting of H, halide, alkyl, substituted alkyl, heteroalkyl, aryl, substituted aryl, and heteroaryl, and where one or more R substituents can be incorporated in a ring structure;

each Z is a substituent independently selected from the group consisting of H, halide, alkyl, substituted alkyl, heteroalkyl, aryl, substituted aryl, and heteroaryl, where one or more of X, Y and/or Z can be incorporated in a ring structure;

M is a polymerizable olefinic monomer;

n is an integer greater than or equal to one, such that $(M)_n$ is polymer derived from one or more olefinic monomer subunits; and

Q^- is a weakly coordinating anion.

7. The compound of claim 6, wherein:

each E is independently selected from the group consisting of N and P;

8. The compound of claim 6, wherein:

each A is independently independently selected from the group consisting of Al, B, Ga, In, Tl, Sc, Y, La and Lu.

9. The compound of claim 6, wherein:

TM is nickel, palladium or platinum.

10. The compound of claim 6, wherein:

TM is nickel, palladium or platinum;

A is aluminum or scandium;

Y is -O-, -S-, or $-CH_2-$;

X is Cl, F, CF_3 or H; and

Z is H.

11. The compound of claim 6, wherein:

$(M)_n$ is a polymer derived from at least one polar functionalized α-olefin.

12. The compound of claim 11, wherein:

the at least one polar functionalized α-olefin is monomer selected from the group consisting of vinyl chloride, vinyl acetate, acrylonitrile, methyl acrylate, methyl methacrylate, methyl vinyl ketone, and chloroprene.

13. The compound of claim 12, wherein:

$(M)_n$ is a copolymer derived from the at least one polar functionalized α-olefin and at least one non-polar α-olefin.

14. The compound of claim 13, wherein:

at least one non-polar α-olefin is selected from the group consisting of ethylene, propylene, butene, styrene, butadiene, and norbornene.

15. A process for polymerizing at least one polar olefinic monomer, comprising:

contacting a catalyst composition according to claim 1 with at least one polar olefinic monomer under polymerization conditions sufficient to polymerize the at least one polar olefinic monomer.

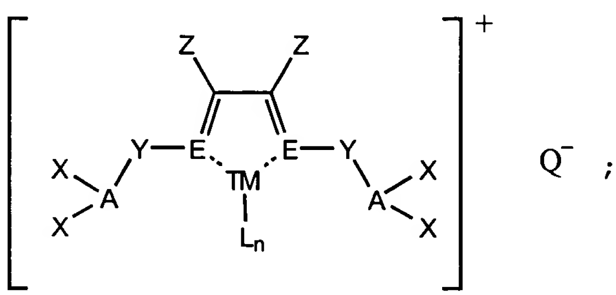
16. A process for polymerizing at least one polar olefinic monomer, comprising:

contacting a catalyst composition according to claim 6 with at least one polar olefinic monomer under polymerization conditions sufficient to polymerize the at least one polar olefinic monomer.

17. A computer-implemented method for identifying polymerization catalyst for a polar olefin, the method comprising:

providing mechanism information for a catalytic polymerization reaction, the mechanism information including electronic data representing a plurality of intermediates and transition states of the catalytic polymerization reaction;

providing a catalyst template, the catalyst template including electronic data representing a catalyst structure characterized by the general formula:



assigning values to each of a plurality of variables representing the components of the catalyst template, such that the values include:

a value for TM representing a late transition metal selected from the group consisting of Groups 7-11 transition metals;

one or more values for E, each representing an electronegative atom capable of donating electrons to the late transition metal;

one or more values for Y, each representing a linking group independently selected from the group consisting of -O-, -NR-, $-CR_2-$, -S-, -PR-, $-SiR_2-$, and $-G(CR_2)_m-$, wherein each R is a substituent independently selected from the group consisting of H, halide, alkyl, substituted alkyl, heteroalkyl, aryl, substituted aryl, and heteroaryl, and wherein one or more R substituents can be incorporated in a ring structure, G is selected from the group consisting of O, N, and CR_2, and m is an integer greater than or equal to 1;

one or more values for A, each representing a Lewis acid;

one or more values for X, each representing an electron-withdrawing group independently selected from the group consisting of Cl, F, Br, I, CF_3, C_6F_5, H, alkyl, C_6H_5, C_6R_5, and CR_3, where each R is a substituent independently selected from the group consisting of H, halide, alkyl, substituted alkyl, heteroalkyl, aryl, substituted aryl, and heteroaryl, and where one or more R substituents can be incorporated in a ring structure;

one or more values for Z, each representing a substituent independently selected from the group consisting of H, halide, alkyl, substituted alkyl, heteroalkyl, aryl, substituted aryl, and heteroaryl, where one or more of X, Y and/or Z can be incorporated in a ring structure;

one or more values for L, representing a plurality of ligands, the plurality of ligands including one or more polarizable monomers, a polymer derived from one or more polarizable monomers, and one or more additional ligands satisfying additional coordination sites of TM or adjusting an oxidation state of TM; and

a value for Q^-, representing a weakly coordinating anion;

systematically varying the values for one or more of TM, A, E, X, Y, or Z to generate a catalyst candidate;

for each of the catalyst candidates, using the mechanism information to calculate a potential energy surface; and

comparing the potential energy surfaces to identify a catalyst for the catalytic polymerization reaction.

18. The method of claim 17, wherein:

systematically varying the values further comprises varying a value representing a solvation energy of the candidate catalysts.

19. The method of claim 17, wherein:

comparing the potential energy surfaces includes performing a screening test for each of a plurality of candidate catalysts, by comparing an energy difference between two or more intermediate structures on the potential energy surfaces for each of the plurality of candidate catalysts, and selecting one or more of the plurality of candidate catalysts for further analysis based on the results of the screening test.